

SPATIAL METHODS IN SCIENCE IMAGE ANALYSIS

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- A. Scientific Inference
- B. Object finding: Volcanoes
- C. Image labeling: Sunspots
- D. Hierarchical and spatiotemporal models
- E. Outlook

Thanks to Michael Burl, Becky Castano, Dennis DeCoste,
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ML FOR SCIENTIFIC INFERENCE

ML methods always give:

Automation: Mechanized process reduces labor and time needed

Cope with increasing data volume (instruments, simulations)

Important for data centers: operations often underfunded

Repeatability: Well-defined algorithm produces results

Uniformity over time key for long-term studies

Allows uniformity among distributed investigators

Crucial for highly charged subjects like climate change

Sometimes one obtains these as well:

Objectivity: Problem-sensitive decision among many conclusions

E.g., model order, number of clusters, which features to use

Often only possible in a limited context or domain

Consensus: Ubiquitous algorithms factor out disagreements

Go beyond ad hoc gadgets to general, cross-domain solutions

Exchange models and algorithms as well as data

Composability: Can analyze machine-generated interpretations

Building a data pipeline, meta-analysis, federated databases

Performance gains are important:

Quality: Quantitative, optimal inference gives better results

Many schemes (implicitly) optimize over interpretations

Gauss obtained the orbit of Ceres by least squares in 1801

Comprehensiveness: Ability to examine more information

Integrate more data within a given interpretation

Achieve total spatial/temporal coverage

GROUND TRUTH — MODEL VALIDITY

Questions brought to fore by scientific problems

Physical questions that seem decidable in principle...

...but whose very intractability motivates inference techniques!

Models for observables

Observables are directly sensed, allowing direct model checks

Can falsify (Popper 1958), but never fully verify

Computing $P(\text{data} \mid \text{model})$ falsifies some models or model classes

E.g., image modeled as three classes, each of which is normal, is falsified if pooled pixels are not a normal three-mixture

Information on hidden variables

This ‘ground truth’ is difficult to come by

- Scientists typically cannot identify objects reliably
 - Problems become very evident at single-pixel scale
 - The most informative test cases are also most uncertain
- Further: Lack of physical understanding of problem means even experts may be surprised at what is really there.

Conceptual inadequacies in models

Methods are often not suitably invariant to resolution

Classes in image segmentation are often not mutually exclusive

Spatial independence is often assumed at some point

Need spatial/temporal stationarity which rarely exists

Bayesian ‘dogma of precision’: every state can be assigned a probability; every outcome can be assigned a cost (Walley 1991)

SPATIAL MODELS

General References

B. D. Ripley, *Statistical Inference for Spatial Processes*, Cambridge, 1988.

Discrete and continuous random fields; morphological operations

N. A. C. Cressie, *Statistics for Spatial Data*, Wiley, 1993.
Especially strong on geostatistics and models for point-sets

Pattern Theory

U. Grenander and Y. Chow and D. Keenan, *Hands: A Pattern-Theoretic Study of Biological Shapes*, Springer, 1991.
A compelling example of synthesis of a complex shape

U. Grenander and M. I. Miller, “Representations of knowledge in complex systems,” *Jour. Roy. Stat. Soc. Ser. B*, 56(4), 549–603, 1994.

Linking abstract models to pixel-level features

Shapes

A. Blake and M. Isard, *Active Contours*, Springer, 1999.
Engineering perspective on parameterizing and tracking boundaries

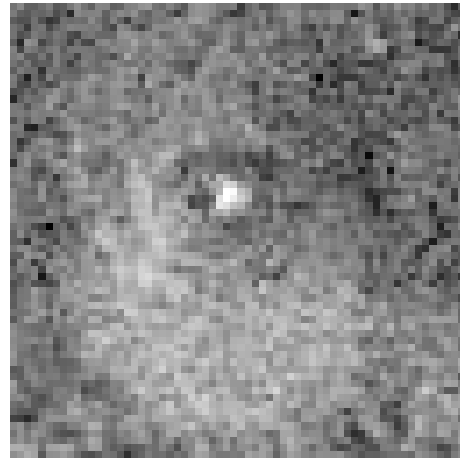
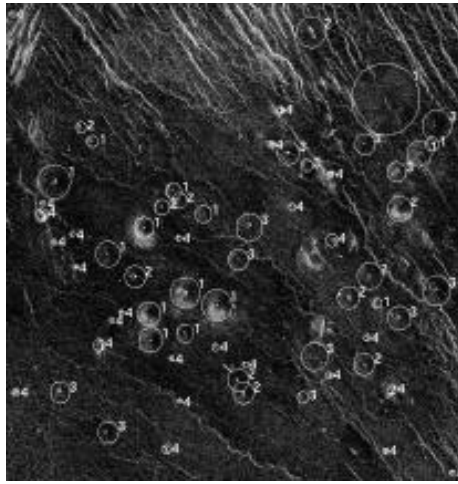
K. V. Mardia and I. L. Dryden, *Statistical Shape Analysis*, Wiley, 1998.

Comprehensive survey of representations and distributions for shapes

OBJECT LOCATION

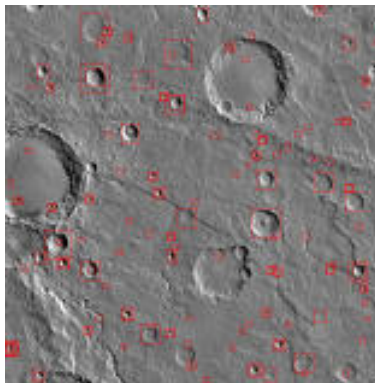
Known object

Example: volcanoes on Venus in SAR imagery from Magellan



Known object family

Example: craters (scale variation; also overlap)



Unknown objects

Potential to detect local variations in a background

LEARNING SCHEME

Due to Michael Burl (JPL) and collaborators
(P. Smyth, U. Fayyad, P. Perona)

To ease computation, all images reduced in resolution 2×2

Two-phase system

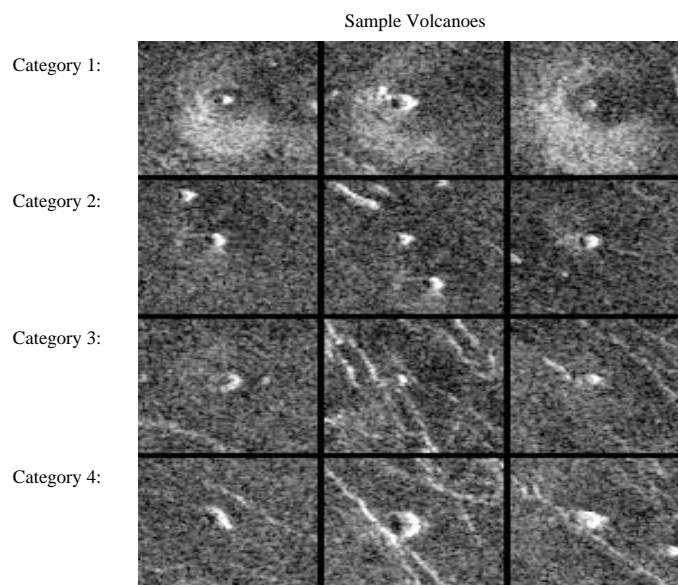
Focus of attention (FOA): Identify all likely candidates

Classification: Assign candidates to classes

FOA sweeps whole image, identifying possible volcano sites which are extracted as square ‘chips’

Classification treats chips as i.i.d. inputs and classes as volcano or non-volcano

Training is done with scientist-supplied training chips.



FOCUS OF ATTENTION

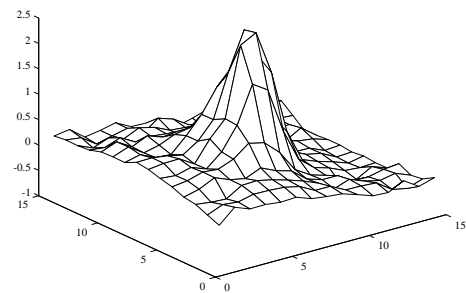
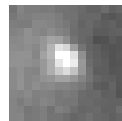
Motivation:

Reduce computation by giving up early on unlikely sites

Allows use of traditional iid classifiers in phase two

Uses scientist-identified volcano sites to find matched filter F

Average of positive examples



F is swept over image to identify strong matches

Less computation by using $F \approx \sum_i f_i f_i^T$

Threshold the correlation to identify potential volcano sites

Sites within four pixels are aggregated in the final list

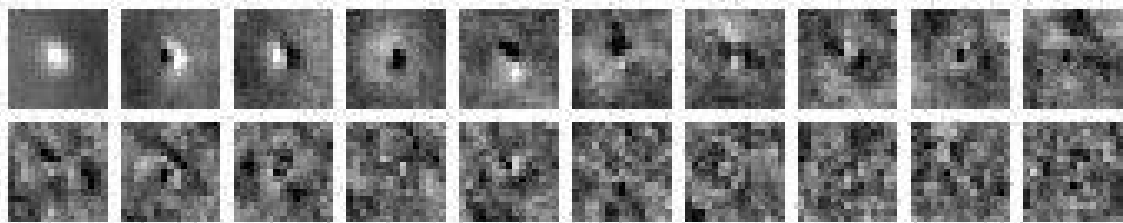
Use family of filters: only limited improvement

CLASSIFICATION

This step is in the realm of classical iid-input algorithms

Non-volcano class is by nature not localized; volcano class is relatively local

Feature selection using PCA compresses 15^2 -dimensional data



Quadratic discriminant analysis forms baseline decision rule

Class-conditional normals with certain mean and covariance

(μ_v, Σ_v) fitted from volcano training data

(μ_{nv}, Σ_{nv}) fitted from non-volcano training data

Classify by thresholding $P(x; \mu_v, \Sigma_v)/P(x; \mu_{nv}, \Sigma_{nv})$

K -Nearest Neighbors a similar-performing alternative

Use all volcano and non-volcano training chips

Majority class among the K neighbors of an input chip wins

Neighbors via weighted Euclidean distance $(x - y)^T R (x - y)$

R chosen to emphasize pixels close to chip center

Resulting accuracy is about as good as human experts in homogeneous data; degrades markedly in heterogeneous regions

Key seems to be to have good information on local non-volcanoes

DIVIDE AND CONQUER

Schema

Method fits relatively well into Dietterich framework

Window, decide, merge

FOA algorithm is where all spatial processing happens

Cleverly, does not choose a fixed window position

Input scale is the 15×15 pixel window

Combination rule: FOA-sites within four pels are aggregated

Output scale is just the granularity of a single volcano

Classification then proceeds independently at each site

Include final V/NV decision into framework as well?

Indicates alternate algorithm where multiple FOA sites are passed through to final classification; then these classes are merged

Fundamental reason this was easy: the discrete, nonoverlapping character of volcanos simplifies the merge

Agenda

Burl et al. 1998: multiple components “make overall system optimization difficult if not impossible given finite training sets”

Optimization seems to enter somewhere, like it or not

IMAGE LABELING

Solar imagery

Reliably identify structures in the photosphere

Sunspots: Depressed intensity and high magnetic flux

Faculae: Regions of enhanced intensity and moderate flux

Quiet sun: everything else

Relate these structures to irradiance changes (weather/climate)

Also: space weather (identify large δ -spots which cause flares)

Mars Geology

Identify soil structure (dust, sand, pebbles)

Detect rocks on soil background

Classify rock types (sedimentary/igneous, weathering, impact)

Methods

Automatic, objective classification using statistical model

Model quantifies the uncertain relation of observables to classes

Model uses spatial information to choose labels

Falsifiable models (Popper 1958) can be checked against
the data they claim to model

General method that extends unchanged to other settings, e.g.
more observables

different number of features

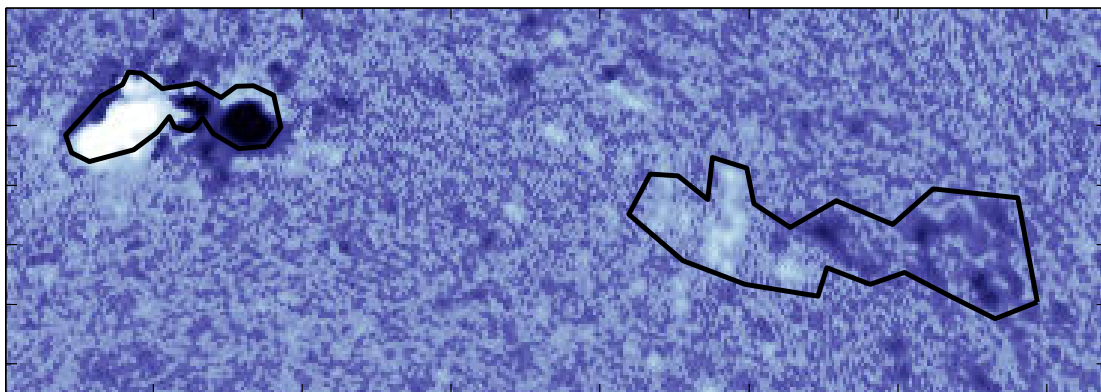
explicit accounting for miscalibration; outliers

inclusion of physical knowledge (like sensor noise)

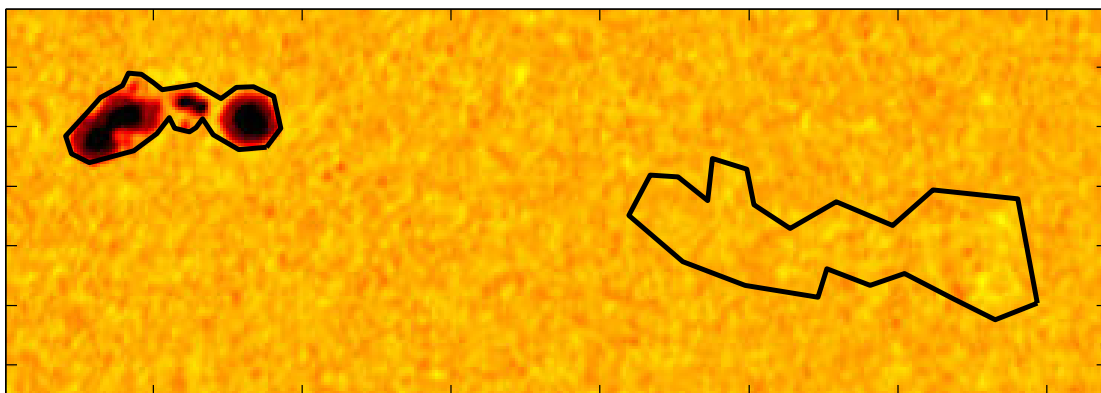
EXAMPLE SOLAR DATA

Irregularly-sampled time series of (full-disk) images
Analyzed May 1996 – Sep 2000; 60 GB across 25 000 images
Below: SoHO/MDI, 17:58 UTC on 7 September 1997

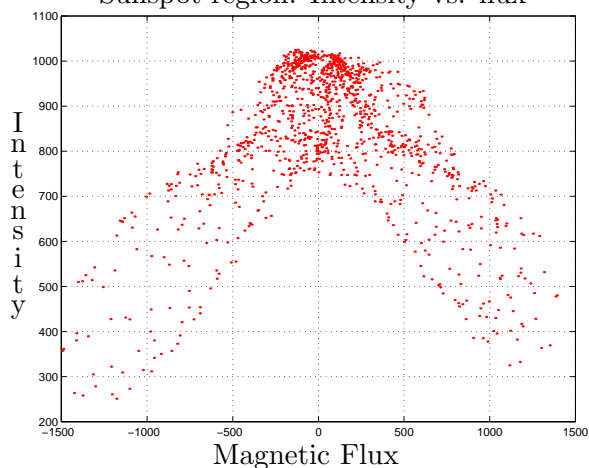
Preprocessed Magnetogram: Detail



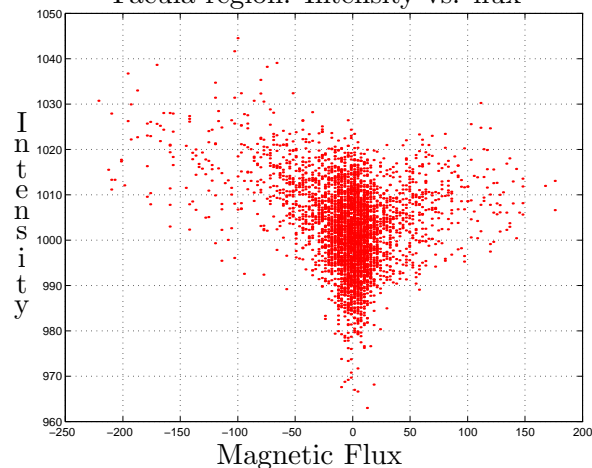
Preprocessed Photogram: Detail



Sunspot region: Intensity vs. flux

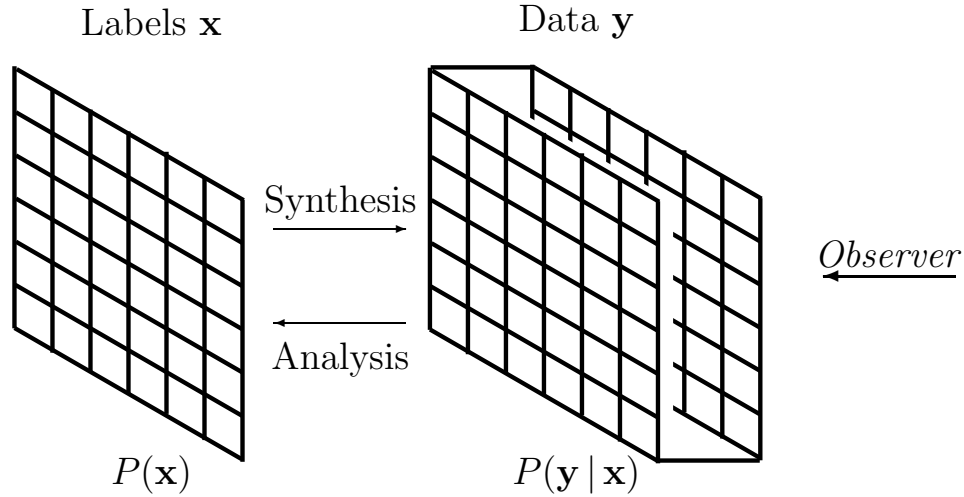


Facula region: Intensity vs. flux



PROBABILISTIC IMAGE MODELS

Quantitatively describe the uncertain relation between observables and labels in a general probabilistic framework



At each spatial position, one of K physical processes is dominant.

Observables arise depending on the dominant physical process.

Generation of observables may be viewed as adding uncertainty (noise) to the underlying dominant process.

Goal of analysis is to invert this noisy mapping.

Variables of the Model

Index set \mathcal{N} of spatial coordinates $s = (i, j)$

Unobservable labels $\mathbf{x} = [x_s]_{s \in \mathcal{N}}$ & observables $\mathbf{y} = [\vec{y}_s]_{s \in \mathcal{N}}$

x_s : small integer $1 \dots K$ (e.g., ACR/Fac/QS)

\vec{y}_s : real vector (e.g., the pair (magnetic field, light intensity))

Statistical model given by two distributions $P(\mathbf{x})$ and $P(\mathbf{y} | \mathbf{x})$

MODEL SPECIFICS: I

Describe the two distributions $P(\mathbf{x})$ and $P(\mathbf{y} | \mathbf{x})$

Linking to Observables with $P(\mathbf{y} | \mathbf{x})$

Make the link via scientist-labeled images and distribution-fitting

Alternatively, can infer automatically from data via clustering

Obtain K distributions, one for each feature class

As strawman, put forward per-class normal distributions

$$P(\vec{y}_s | x_s = k) \sim \text{Normal}(\vec{\mu}_k, \Sigma_k)$$

with $d \times 1$ class means and $d \times d$ covariance matrices.

(QS class, $k = 1$: fits the SoHO/MDI data reasonably well using $\vec{\mu}_1 = [0 \ 1]$ and $\Sigma_1 = (0.01)^2 I$.)

For MDI, the normal distribution is inadequate for all classes:

strongly multimodal

cannot even transform to normality (e.g., with $|\text{flux}|$)

quiet class, e.g., contains superpositions of effects

(supergranulation is discernable in scatter plots)

\implies it fails standard statistical tests.

...normal model is thus *falsified*.

We must introduce more realistic data models $P(\vec{y} | x)$

MODEL SPECIFICS: II

Quantifying Spatial Smoothness with $P(\mathbf{x})$

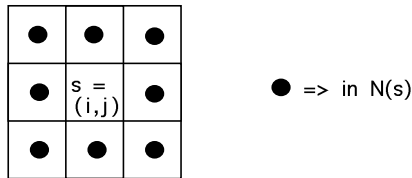
Typically $\beta \geq 0$ controls smoothness in the prior

$$P(\mathbf{x}) = \frac{1}{Z} \exp\left(-\beta \sum_{s \sim s'} 1(x_s \neq x_{s'})\right)$$

where $s \sim s'$ means: site s close to site s' , e.g. one pixel away

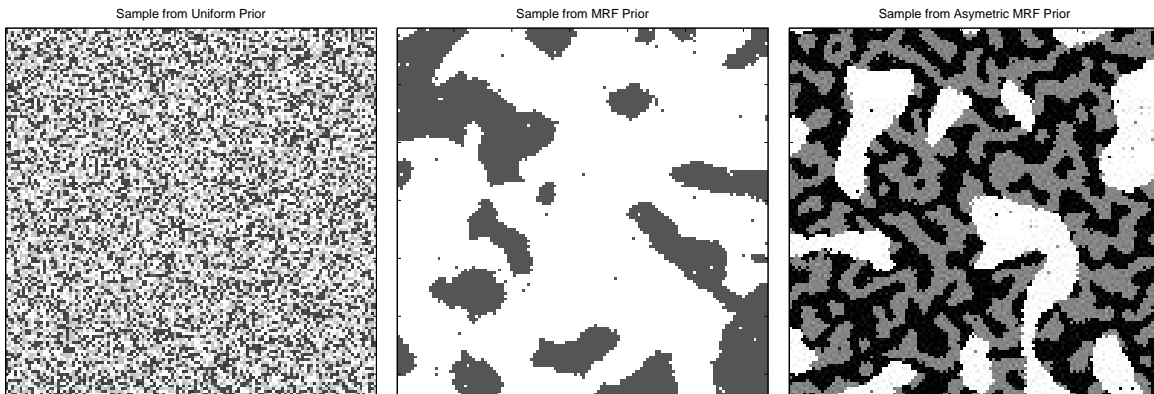
Penalty of β per disagreement of nearby pixels to enforce spatial coherence of labelings

Key property of locality: $P(x_s = x \mid x_{(s)}) = P(x_s = x \mid x_{\mathcal{N}(s)})$



At $\beta = 0$, penalty and spatial constraint vanish

Sample realizations from $P(\mathbf{x})$



ASIDE: CONTINUITY AND EDGES

Such Markov random field models allow edges in modeled images

Change in discrete hidden variable forces

significant change in real-valued observable

Jumps undesirable in typical image *restoration* contexts

Motivates conditional autoregressive (CAR) model

$$P(x_s = x \mid x_{(s)}) = P(x_s = x \mid x_{\mathcal{N}(s)}) = N(Ax_{\mathcal{N}(s)}, \Sigma)$$

but with conditionally normal distribution

(Autoregression: predict x_s in terms of “itself” $x_{\mathcal{N}(s)}$)

Joint distribution of CAR model is normal, easing computation

Natural parallel with familiar one-dimensional models

	Continuous	Discrete
Time Series	Autoregressive (AR) or Kalman models	Hidden Markov models (HMM)
Imagery	CAR models	Markov random fields (MRF)

MRF computations are the hardest: our best tools do not apply

Non-gaussian, so no reduction to clever matrix manipulations

Bayes net of many short cycles, junction tree algs liable to fail

But: sampling, Metropolis-Hastings, and MCMC methods

developed for MRFs enable very complex models

SIMULATING MRFS

Distribution $P(\mathbf{x}) = Z^{-1} \exp\left(-\beta \sum_{s \sim s'} 1(x_s \neq x_{s'})\right)$

No direct simulation: no Z , and state space of \mathbf{x} huge!

Randomized algorithm: Gibbs sampler

Basis: craft a MC having P as its stationary distribution

Adaptation of stat-mech methods (c.f. Metropolis *et al.* 1953)
for simulating the state of interacting systems

Iterative algorithm: starts at some labeling and
refines it pixel-by-pixel over many image sweeps

Method:

Choose an initial $\hat{\mathbf{x}}$

Scan pels in raster fashion.

At pel s , find $P(\hat{x}_s = x \mid \hat{x}_{(s)}), 1 \leq x \leq K$. [*]

Choose new \hat{x}_s by drawing from this distribution

Repeat scanning

Result: As scans go to infinity, $\hat{\mathbf{x}} \Rightarrow P(\cdot)$.

That is, iterate enough and the labeling is a draw from $P(\mathbf{x})$

Remarks

Note local combination rule [*]

Flip of one label can eventually influence all labels

This method, and similar Metropolis-Hastings methods, are the
basis for updating more complex spatial models

INFERRING THE LABELING

Invert the noisy data via *maximum a posteriori* (MAP) rule

$$\hat{\mathbf{x}} = \arg \max_{\mathbf{x}} P(\mathbf{x}|\mathbf{y})$$

Bayes formula shows $P(\mathbf{x}|\mathbf{y}) \propto P(\mathbf{y}|\mathbf{x})P(\mathbf{x})$

For normal $P(y_s | x_s)$, algebra reveals the objective function

$$\log P(\mathbf{x}|\mathbf{y}) = -\frac{1}{2\sigma^2} \sum_{s \in \mathcal{N}} \|\vec{y}_s - \vec{\mu}_{x_s}\|^2 - \beta \sum_{s \sim s'} 1(x_s \neq x_{s'})$$

Interpretation

First term: fidelity to data (observation close to its mean)

Second term: image smoothness (this couples the pixel labels)

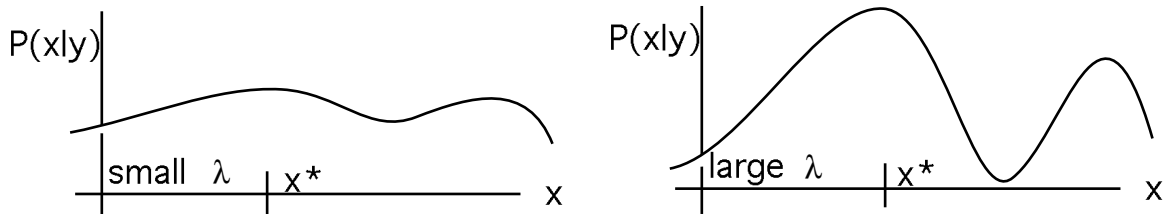
Maximizing $P(\mathbf{x} | \mathbf{y})$

- Use Gibbs sampler to *draw* from the distribution $P(\mathbf{x} | \mathbf{y})$
- To *maximize* $P(\mathbf{x} | \mathbf{y})$, nest G.S. within simulated annealing
That is, pick large λ and draw via G.S. from

$$P_\lambda(\mathbf{x} | \mathbf{y}) := (1/Z_\lambda) P(\mathbf{x} | \mathbf{y})^\lambda$$

(Effectively scale entire log-posterior, above, by λ)

- Simulated annealing: raise λ as Gibbs sampler iterates
If λ up slowly enough, mode is reached



- Takes about 3 min/image on Sun workstation (360MHz).

MODELING THE OBSERVABLES

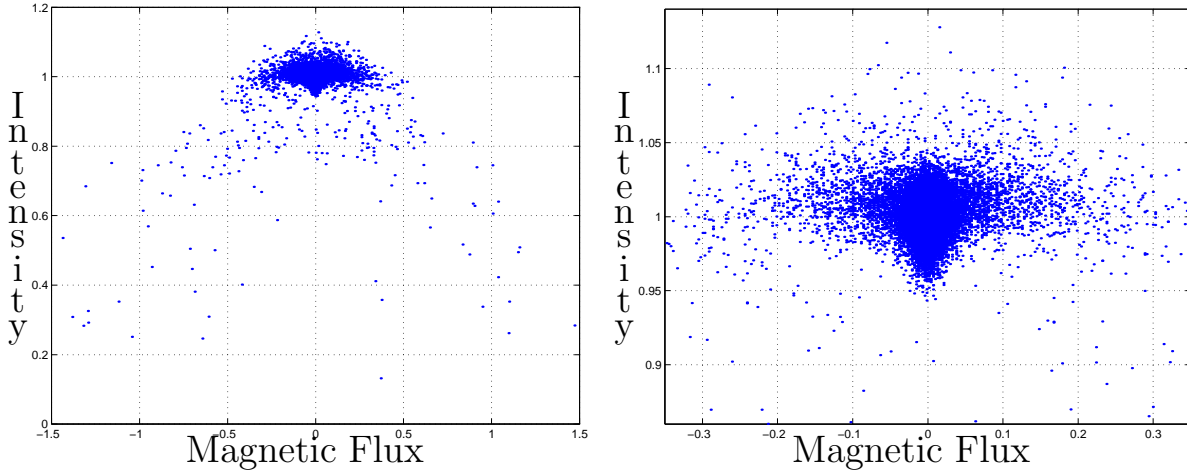
For realistic models, benefit from the flexible mixture density

$$p(\vec{y}; \theta) = \sum_{g=1}^G \alpha_g N(\vec{y}; \vec{\mu}_g, \Sigma_g)$$

$$\theta = \{(\alpha_1, \vec{\mu}_1, \Sigma_1) \cdots (\alpha_G, \vec{\mu}_G, \Sigma_G)\}$$

Accounts for multimodality and superpositions of effects

A very general family: take G large.



Ask scientists to find regions of type $x_s = k$; estimate θ_k for each

Goal: From data $Y = [\vec{y}^1 \cdots \vec{y}^n]$, find a density model $p(\vec{y}; \hat{\theta})$

Method: Determine parameters by maximum-likelihood using Y :

$$\hat{\theta} = \arg \max_{\theta} \log P(Y; \theta) = \arg \max_{\theta} \sum_{i=1}^n \log p(\vec{y}^i; \theta)$$

Performed via EM algorithm: done once and the model is fixed

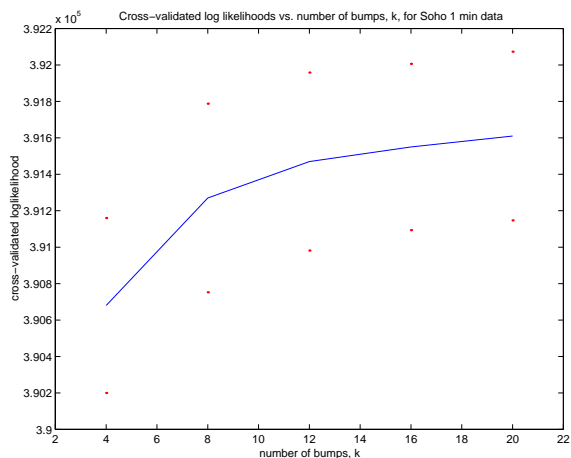
Unsupervised mode: Provide cumulative data over classes, and

EM clusters \vec{y} into classes: clusters are extracted after the fact.

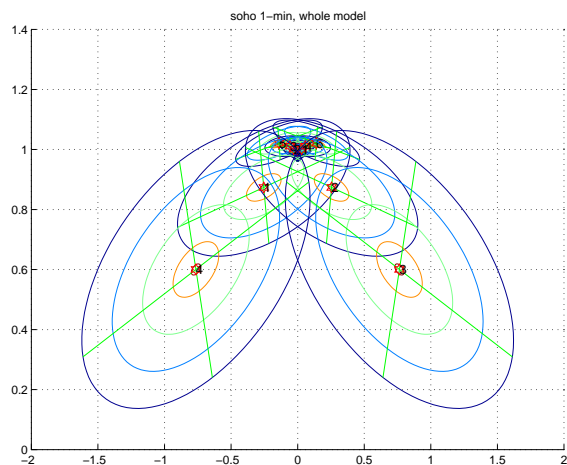
Order selection by cross-validated likelihood (Smyth 1999)

MODELS USED: SOHO/MDI

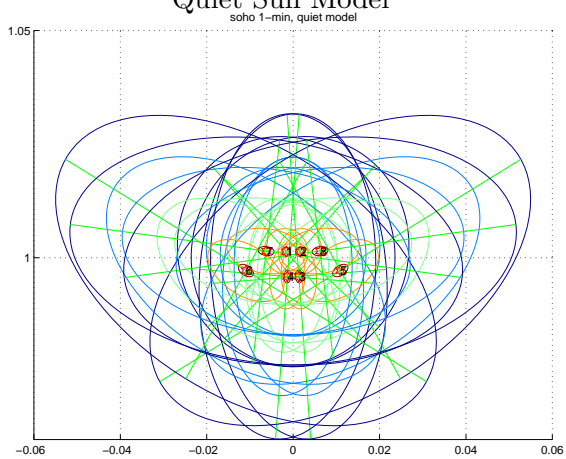
Model Fit, varying Complexity



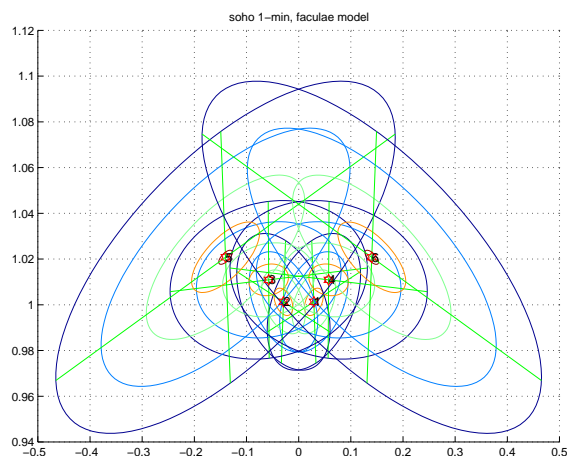
Entire Model



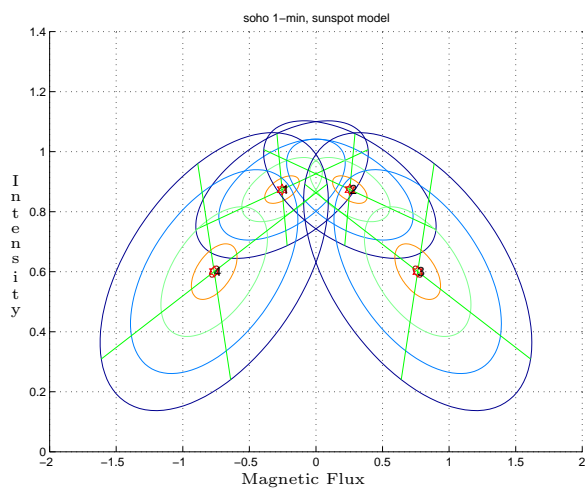
Quiet Sun Model



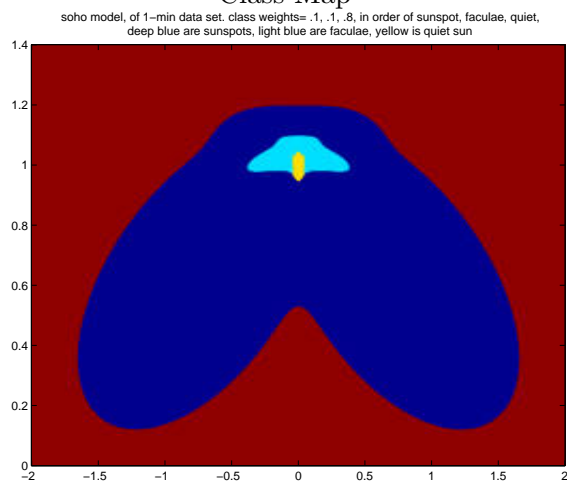
Facula Model



Spot Model

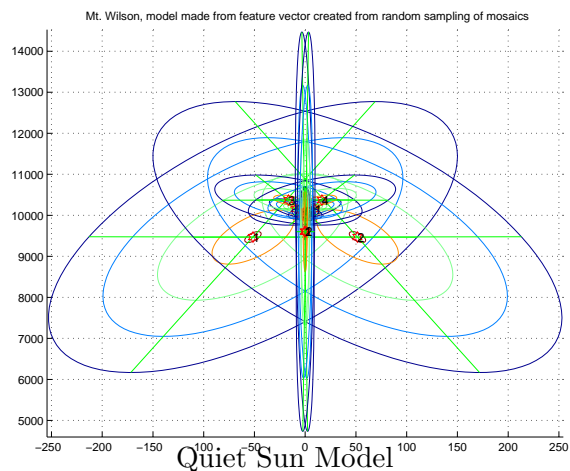


Class Map

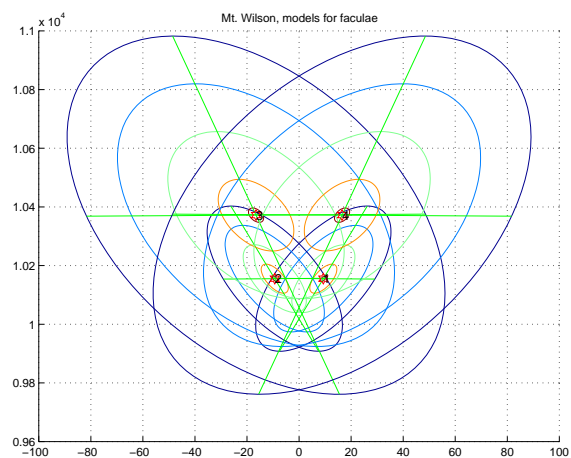
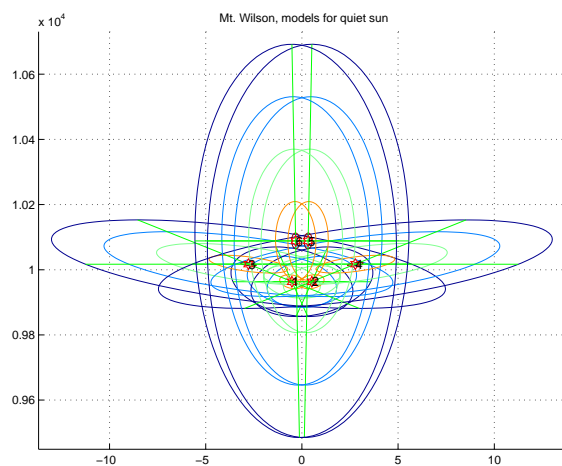
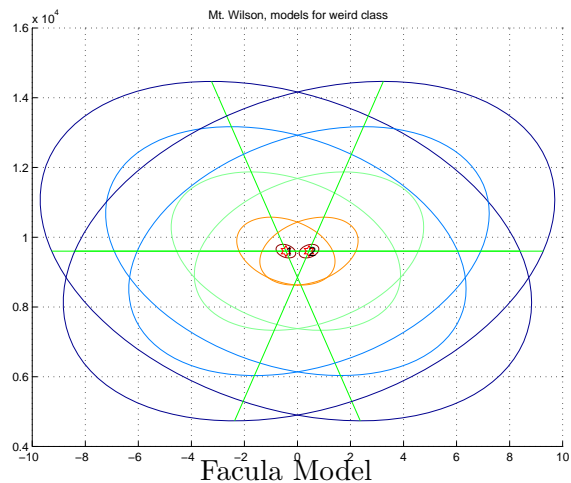


MODELS USED: MT. WILSON

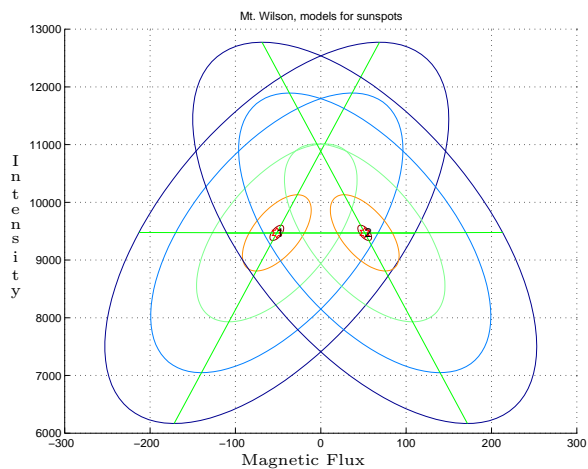
Entire Model



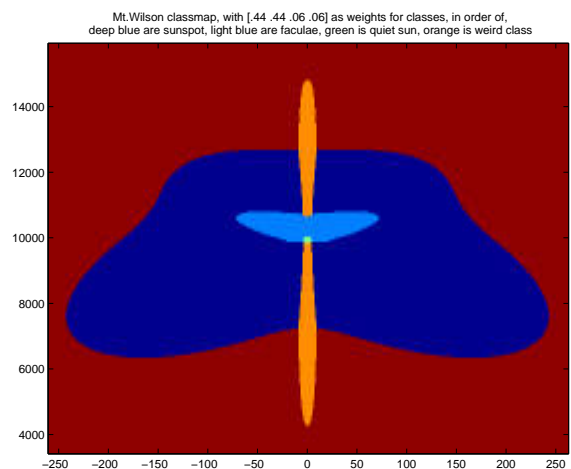
Miscalibration Model



Spot Model

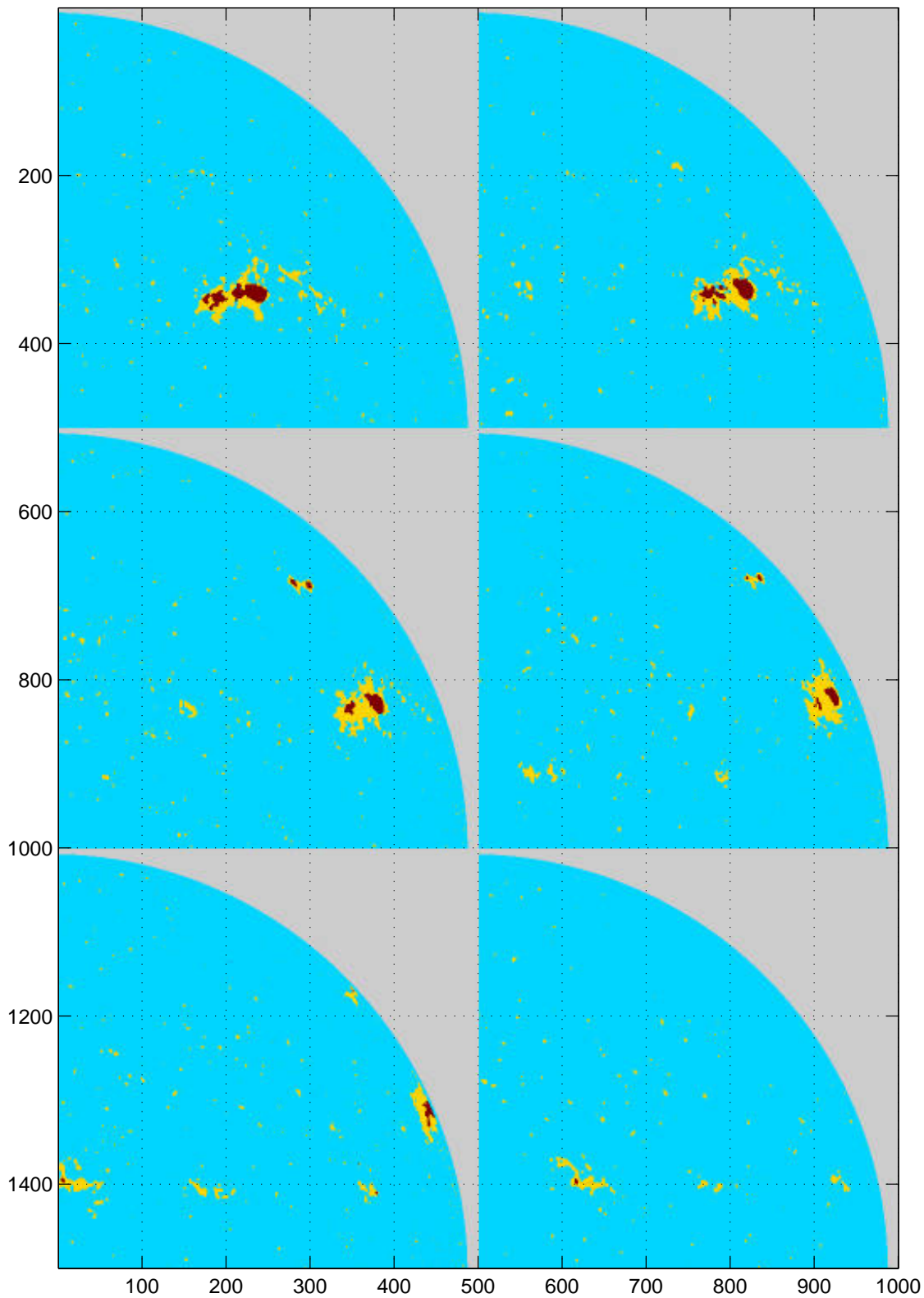


Class Map



LABELINGS

Labeling: 1998/01/15 11:11 UTC + 0,1,2,3,4,5 days



HIERARCHICAL SPATIAL MODELS

Better Representations

Represent an object via a *compactly-described* membership function h_s indicating subjective belief site s is active region

- Larger-scale representation of an object
- Provides interpretability

Several Simple Mechanisms

Outlines: Grenander et al., 1991

Polygons: Green 1996

Continuum triangulations: Nicholls 1997, 1998

Delaunay triangulations: Turmon 1998

Binds nearby on-object regions into one object

Two fundamental quantities:

Indicator function h_s , $s \in \mathcal{N}$

$h(s) = 1$ means on-object, $h(s) = 0$ if not

Parameterized by tie points in \mathcal{N} .

Function complexity $\kappa(h) \geq 0$

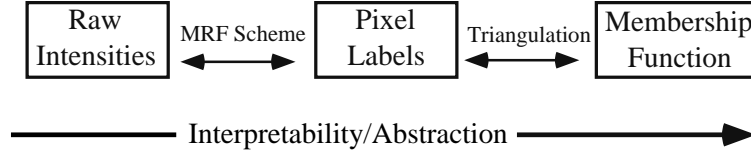
e.g., the number of tie points, or

intensity of point process generating tie points

LINK TO OBSERVATIONS

Establish Markov dependence between hierarchical model layers

$$P(h, \mathbf{x}, \mathbf{y}) = P(h)P(\mathbf{x} | h)P(\mathbf{y} | \mathbf{x})$$



Probabilistic Model

Penalize complexity by setting

$$P(h) = Z^{-1} \exp[-\gamma \kappa(h)]$$

This choice gives an additive penalty to disjoint objects

Intermediate layer uses h_s to bias the event $\{x_s = \text{Object}\}$:

$$-\log P(\mathbf{x} | h) = \beta \sum_{s \sim s'} 1(x_s \neq x_{s'}) + \alpha \sum_{s \in \mathcal{N}} |1(x_s = \text{Object}) - h(s)|$$

The data distribution $P(\mathbf{y} | \mathbf{x})$ is as before.

- One can do inference by maximizing the posterior

$$P(h, \mathbf{x} | \mathbf{y}) = P(h, \mathbf{x}, \mathbf{y}) / P(\mathbf{y}) \propto P(h, \mathbf{x}, \mathbf{y})$$

or minimizing its negative logarithm

$$\begin{aligned} & \gamma \kappa(h) + \alpha \sum_{s \in \mathcal{N}} |1(x_s = \text{Object}) - h(s)| \\ & + \beta \sum_{s \sim s'} 1(x_s \neq x_{s'}) + \frac{1}{2\sigma^2} \sum_{s \in \mathcal{N}} (y_s - \mu_{x_s})^2 \end{aligned}$$

INFERRING COMPLEX MODELS

We describe inferring shape models for fixed labeling

To speed convergence, replace $1(x_s = \texttt{Object})$ above with its probability given the data

(Fully analogous to ICE algorithm of Art Owen)

Now the objective simplifies to

$$\gamma \kappa(h) + \alpha \sum_{s \in \mathcal{N}} \left| P(x_s = \texttt{Object} \mid \mathbf{y}) - h(s) \right|$$

Metropolis-Hastings sampler

Inference means choosing tie-point positions

Construct a Markov chain on the state space of tie points

$$\mathcal{V} = \bigcup_k \mathcal{V}_k = \bigcup_k (\mathcal{N} \times \mathcal{N})^k$$

that has limit distribution

$$\pi(h) = P(h \mid \mathbf{x}, \mathbf{y})$$

(Maximize $P(h \mid \mathbf{x}, \mathbf{y})$ with same annealing setup as earlier)

Metropolis-Hastings proposes state changes and probabilistically accepts them to achieve the desired limit distribution

The operator set consists of

- tie-point move (M),
- tie-point raise/lower (R),
- tie-point add (A_k) or kill (A'_k)

SPATIO-TEMPORAL INFERENCE

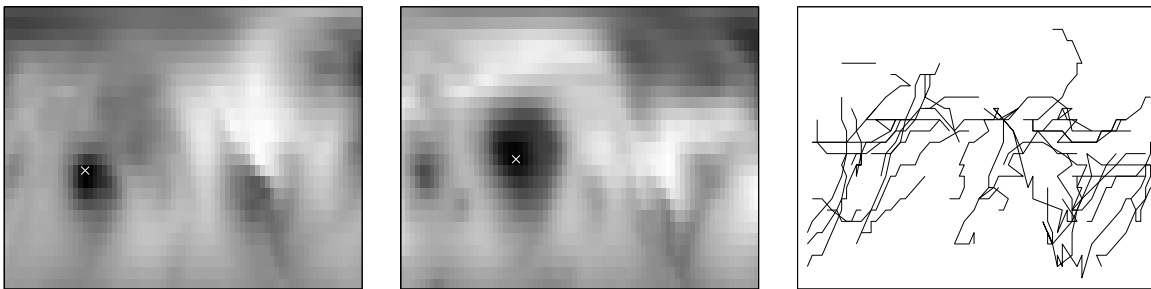
Object trajectories

Sea-level pressure over the Pacific ($\delta t = 48$ hrs.)

Cyclone center shown by white cross

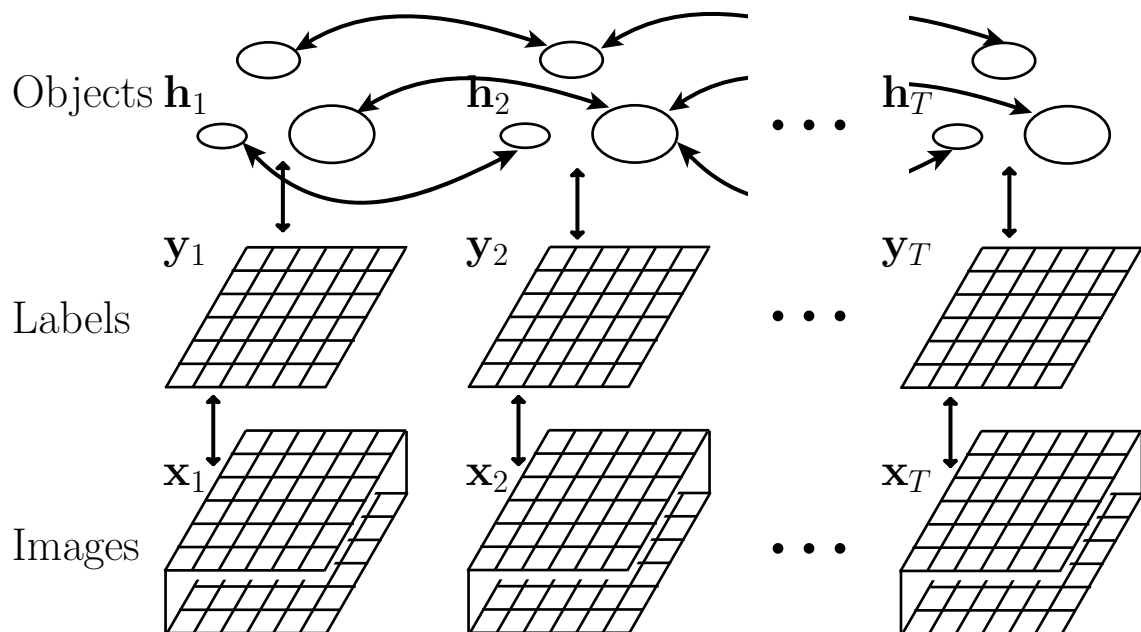
Right: trajectories from a series of (quantized) observations

Data from P. Smyth, UC Irvine



Other examples: sunspot motion, microblock motion from GPS

Objects through time



MODELING THE TEMPORAL PART

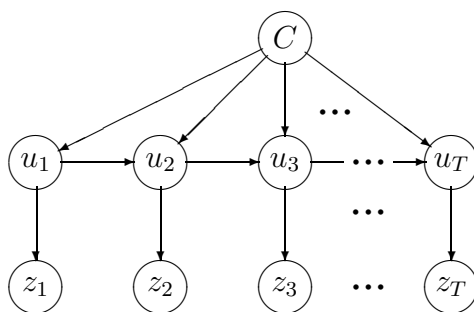
State-based motion models

Include influence of exogenous inputs and observable covariates

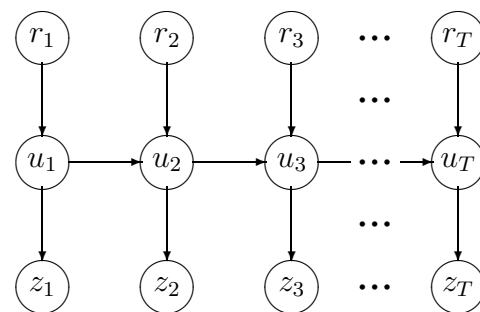
Discover motion clusters by uncovering a hidden class C

Examples

Generalizations of the Kalman filter as Bayes nets with state u_t



mixed dynamical model



model with exogenous inputs r_t

Build temporal models atop de-coupled spatial models

Implications

Two domains of divide and conquer

Easy cases: dominant locality in space (sunspots) or time (GPS)

...allows decoupled solutions

Coping with both simultaneously is harder, even beyond current limits of practical optimization technology

Problems...

estimate model parameters automatically

learn the model structure automatically

SPATIO-TEMPORAL MODELING (I)

Base concept of random vector is inadequate

Capture concept of variables on structured index sets

Domain : An index set

- Principal Examples:

Any finite set

Z_n , the first n integers (e.g., time series)

Z/Z_n , the cyclic version of Z_n

R , the real numbers

Domains supporting translation play a special role

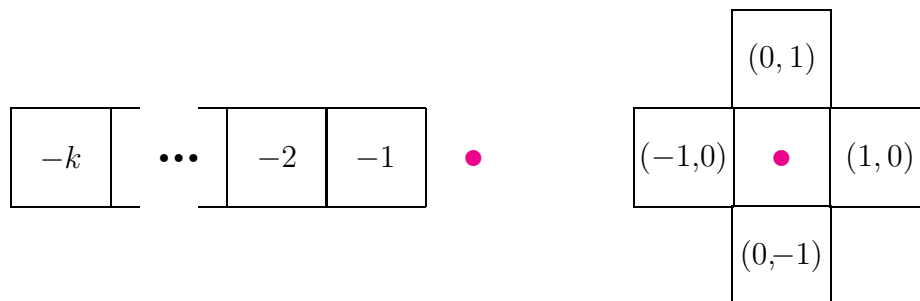
- Operators on domains give means of combination

\cup , the union

\times , the cross-product

Allows formation of domains for images, etc.

- Stencil* is a Domain identifying a local neighborhood
 $\{-k, \dots, -2, -1\}$, for a k -order autoregressive model
 $\{(-1, 0), (1, 0), (0, -1), (0, 1)\}$, for a first-order MRF



SPATIO-TEMPORAL MODELING (II)

Field : Mapping on a Domain

Random Field a mapping from a Domain to earlier Variables
...the spatiotemporal generalization of random variable

Principal examples:

Time series are random fields over Z or R

Multispectral images: random fields over $\times(\{1, \dots, k\}, Z_n, Z_n)$
(spectral index does not support translation)

Neighborhood a Field from (Domain, Stencil) to a Domain

...maps (site, offset) \mapsto site', often by translation

...supports *adjacency* for dependence structures

Let M be the neighborhood corresponding to the order-1 MRF

Then $M(i, k)$ is the k -th neighbor of site i

$M(i)$ is the set of all neighbors of site i

unpack operator

...returns the neighborhood M given a Domain and Stencil

MODEL SPECIFICATION

- Simplest models have no conditional dependence:

$$\mathcal{D} = Z_n$$

$$(\forall i \in \mathcal{D}) x[i] \sim \text{Normal}(i, 4)$$

- AR model:

$$\mathcal{D} = Z_n$$

$$\mathcal{S} = -1$$

$$M = \text{unpack}(\mathcal{D}, \mathcal{S})$$

$$(\forall i \in \mathcal{D}) x[i] \sim \text{Normal}(x[M(i; -1)], 1)$$

- The standard Potts MRF prior:

$$\mathcal{D} = \times(Z_n, Z_n)$$

$$\mathcal{S} = \{(-1, 0), (1, 0), (0, -1), (0, 1)\}$$

$$M = \text{unpack}(\mathcal{D}, \mathcal{S})$$

$$(\forall i \in \mathcal{D}) ct[i] = \sum_{k \in M(i)} x[M(i; k)]$$

$$(\forall i \in \mathcal{D}) x[i] \sim \text{Discrete}\left(0, \frac{e^{ct[i]-4}}{e^{ct[i]-4} + e^{-ct[i]}}, 1, \frac{e^{-ct[i]}}{e^{ct[i]-4} + e^{-ct[i]}}\right)$$

Import just enough mathematical notation to express the models

CONCLUSIONS

Machine procedures offer many benefits to scientific inference

Persistent issues:

- Building tractable models of observational reality

- Obtaining accurate training data

- Designing and executing clear falsification experiments

Finding Objects

Discussed a good algorithm-based approach

Divide and conquer schema applicable (even suggestive) here

Labeling Images

Use of statistical models allows falsification experiments,

- easy extension to wider class of problems

Spatially, temporally uniform data is key to accurate labelings

Complex models

Useable temporal and spatial statistical models do exist

...but the best ML perspectives often absent from this work

- agnostic models, robust algorithms, cross-validation, automation

Cooperating space/time models, linked spatiotemporal models

Futures

Object-level recognition in non-algorithmic framework

Languages to express statistical models on structured domains

Model selection in complex, flexible model space